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Exposure Assessment Modeling A State-of-the-Art Review

John F Kennedy School of Government, Cambridge, MA

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Exposure Assessment Modeling

A State-of-the-Art Review

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EXPOSURE ASSESSMENT MODELING:
A STATE-OF-THE-ART REVIEW

by

Catherine Miller
Kennedy School of Government
Harvard University
Cambridge, Massachusetts 02138

Grant No. 805647

Project Officer

Kenneth Hedden
Technology Development and Applications Branch
Environmental Research Laboratory
Athens, Georgia 30605

ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ATHENS, GEORGIA 30605

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FOREWORD

Environmental protection efforts are increasingly directed towards preventing adverse health and ecological effects associated with specific compounds of natural or human origin. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Technology Development and Applications Branch develops and evaluates management or engineering tools for assessing and controlling adverse environmental effects of these substances.

Solutions to serious environmental pollution problems increasingly involve analyzing and evaluating difficult trade-offs between useful substances and products and risks posed to human health and environmental quality from toxic materials. One useful method for estimating the actual human and environmental exposure to substances and their effects is the application of mathematical models. This report investigates a number of multimedia mathematical exposure assessment models now in use or under development and provides recommendations for research priorities in the further development of these techniques for the use of environmental decision-makers.

David W. Duttweiler
Director
Environmental Research Laboratory
Athens, Georgia

ABSTRACT

This report presents a state-of-the-art review of exposure assessment modeling. It describes currently available models that simulate the environmental fate of substances, the exposure to such substances, and the effects of such exposure. The focus is first on exposure and effects, where relatively little work has been done, and then on models of environmental fate, in particular on intermedia transfer processes. Single-medium air and water quality transport models are not assessed, but the possibility of approaching multi-media problems through a combination of single-medium approaches is explored. The report also describes several actual risk assessments that have been made with limited data, and considers some secondary applications of the models that have been suggested.

The results of this investigation show that the available models do not cover all of the areas necessary for an exposure assessment. More effort has been directed to modeling environmental fate than to modeling exposure and effects.

In general the models are not operational from the decision-maker's point of view because they have not been validated, lack sensitivity analyses for key parameters, do not include cost estimates and often call for data not readily available. There are also organizational and administrative barriers to the actual use of these models.

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CONTENTS

Foreword	iii
Abstract	iv
Acknowledgments	vi
I. Introduction	1
II. Conclusions	4
III. Recommendations	7
IV. Modeling Exposure and Effects	9
Health Effects	9
Dose-response Relationships	11
Ecological Modeling	13
Human Population Exposure	16
Summary	17
V. Modeling Interfaces between Media	19
Air and Soil/Water Interface	20
Source Depletion Model	21
Surface Depletion Model	21
Wet Deposition Rates	22
Dry Deposition Rates	23
Evaporation or Volatilization Rates	23
Soil and Water Interface	26
Adsorption-desorption	27
Transport from soil to aquatic systems	28
Uptake in Biological Systems	29
Summary	30
VI. Examples of Fate Models	32
Unified Transport Model	32
Conceptual Model	37
Mass Balance Approach	38
Environmental Rates Approach	40
Summary of Fate Model Findings	43
VII. Examples of Exposure Assessments	45
VIII. Other Uses for the Models	48
Integrated Exposure Assessment Monitoring	48
Ranking Schemes	49
IX. References	51

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SECTION I

INTRODUCTION

Recent events in the environmental protection field have demonstrated that the first generation of control activity has run its course. Solving the more serious problems that remain will require a much greater degree of understanding and sophistication, particularly in analyzing and evaluating the desirability of alternative actions. In the future, we will be faced with difficult trade-offs between useful substances and products and the concomitant risks posed to human health and environmental quality.

In the past, EPA's approach has been to model sources of pollutants and apply controls to these sources. Single-medium models have been used to simulate changes in air or water quality due to substances emitted or discharged directly into the medium being modeled. Quality is described in terms of concentrations, spatially and/or temporally determined. However, simply knowing where and how a potential pollutant is being released to the environment is not an adequate basis for making the sort of trade-off decisions that will be required. It is also necessary to estimate the actual human and environmental exposures and the effects that result from these exposures.

In assessing exposure, the decision-maker needs information on:

- transport, transformation and fate of the substances through all the media
- exposure of humans, animals and plants to the substance
- effects on humans, animals and plants
- severity and likelihood of occurrence of the effects.

This information can be supplied in a variety of ways; mathematical models may be one of the most useful.

A model is a tool for exploring complex phenomena and their interactions. It is a simplified representation of the interrelationships among elements of the particular system to be explored. A model can take various forms. It can be a purely mental model or philosophical construct. Explicit models include schematic ones, such as blueprints; physical ones, such as microcosms; and symbolic ones. The models we investigate in

this paper are symbolic, and use equations to represent the interrelationships. A mathematical model expresses symbolically one or more elements of the system (dependent variables) in terms of the others (independent variables). The decision-maker uses the model to predict what will happen to certain elements of the system when the independent variables are varied or controlled. These predictions, e.g., severity and likelihood of a particular effect from a given change in pollutant emissions, can provide a basis for setting priorities and making trade-off decisions. Basically, they detail the range of outcomes that is available given alternative control strategies.

As mentioned above, the mathematical model is only one of a variety of ways to provide the necessary information. Other methods include monitoring and field and laboratory experiments. Whether the decision-maker will use a model and which model he will use will depend on the accuracy of its representation of the system being studied and on how easily, and at what cost, it provides the needed information. More specifically, the decision-maker's criteria for evaluating the usefulness of a model would include:

- applicability (appropriate boundaries, outputs useful for the particular problem)
- accuracy of estimates and validation of model
- whether necessary data inputs are available
 - assumptions explicit and significance of results explained
 - sensitivity analyses
- cost compared to other studies or sources of information.

Clearly these criteria are interrelated. In many situations they are competitive and trade-offs among them will have to be made.

The application of these criteria raises several specific issues that must be addressed in a state-of-the-art assessment of this type of modeling. The first issue concerns applicability. In exposure assessment, a useful model should represent important chemical, physical and biological processes and interactive (synergistic or antagonistic) effects for each medium. In addition it should produce estimates of the environmental fate of substances, exposure and effects across media.

The second issue concerns accuracy, comprehensibility and other operational aspects of the criteria. It is important to hold down the cost of collecting input data and running the model, if it is to be used. Regardless of the model's simplicity or accuracy, the decision-maker will not use it if he does not understand what its results mean.

The third issue concerns actual use. Given the complementary nature of the criteria, models of varying degrees of

applicability and operational readiness will or will not be used in particular situations. Thus, the actual model uses and the circumstances surrounding their use are also an important part of a state-of-the-art assessment.

This report investigates a number of mathematical exposure assessment models now in use or under development, considering the completeness with which they cover the phenomena of interest, their practical operational qualities, and the particular uses to which they have actually been put.

Because, fundamentally, we are most concerned with the effect of substances on human beings, those models that incorporate exposure and effects are discussed first. These include studies of health effects, ecological modeling and human population exposure studies.

These models depend on estimates of pollutant concentration levels. Because of the single-medium focus of control activities mandated by U.S. environmental legislation and EPA's historical approach to regulation, a large number of models exist to predict such concentrations in particular media. Assessing these single-medium models is beyond the scope of this report. Such models could be useful in assessing exposure if linked together in such a way as to account for intermedia fluxes, however. This report characterizes the information needed to link together single-medium transport and transformation models, and gives examples of a sequentially linked model and other approaches to studying environmental fate.

The final sections of the report present examples of exposure assessments that have been made and discuss other uses for the information provided by the models described in this report.

SECTION II

CONCLUSIONS

Three issues have been investigated in this state-of-the-art assessment of exposure assessment modeling: applicability or coverage, operational state, and actual use of the models for decision-making. Specific conclusions regarding these three issues are summarized here.

APPLICABILITY

Available models have not given equal attention to the various factors that should be of concern in an exposure assessment. Population exposure and interactive effects (synergistic or antagonistic) are the least understood or studied. The vast majority of models deal only with a single pollutant and do not consider possible interactive effects with other pollutants.

Only rather primitive studies of population exposure have been done so far. These studies have been limited by their dependence on census data of residential living patterns for the human population. In addition, no sound theoretical basis has been produced for developing predictions based on actual behavior patterns, including travel and work.

Ecological models for plant and animal populations also suffer from a lack of unifying theories for biological interactions and thus tend to be highly site-specific, not permitting extrapolation. In addition, because they often fail to estimate both the level and the duration of exposure, the quantitative link from dose to response frequently cannot be made.

Information on effects comes mainly from experimental tests or field (epidemiologic) studies. Theoretically, it can be linked to environmental fate and exposure models through a dose-response relationship. Extrapolating from tests done on one species (animal) to another species (human) is inherently problematic, however. Moreover, experimental doses frequently do not correspond to low environmental concentrations. Finally, epidemiologic studies record correlations but rarely are able to specify cause and effect; thus findings from such studies should not be accepted uncritically for use in exposure assessment models.

Models do exist for studying transport and environmental fate, though their applications remain largely single-medium oriented. Moreover, they are most appropriately used for conservative or non-reactive substances, because models of chemical and biological transformations are not as advanced as models of physical transport. Advances have been made in modeling chemical processes, which predominate in the air medium, however. Without a theoretical knowledge of the underlying processes, water and soil models remain dependent on empirical estimation of parameters describing the distribution of pollutants.

This report focuses on models of the processes at the interfaces between the media. Here again, little is known of the fundamental mechanisms underlying these processes. Accordingly, models characteristically rely on empirical estimates of parameters and require large input data sets and calibration for specific sites before use. Several conceptual approaches to modeling environmental fate from a multi-media perspective have been suggested, but only a few actual applications exist. Thus, verification or experience with which to choose among the alternative approaches is lacking.

OPERATIONAL CAPABILITY

Far more models have been proposed than are currently operational. The relative abundance of suggested approaches and paucity of applications is due in part to irrelevant or inadequate data. The models' data requirements are beyond available resources or in some cases beyond measurement capability. In order to use a model, the decision-maker must also understand its assumptions and the significance of its results. Generally, these foundations of a particular model are well documented. However, in almost no case is the model's accuracy, sensitivity to key parameters, or cost defined. This information must be available to the decision-maker if the model is to be considered truly operational.

ACTUAL USE

Problems of organization and administration exacerbate these technical problems and act as a barrier to the actual use of the models. An exposure assessment requires a combination of skills traditionally taught and practiced separately. Usually health effects researchers are not trained in chemistry and chemists know little biology, so that interdisciplinary teams must be formed to develop the model. Within EPA, modelers are not generally working with those responsible for monitoring systems, so that coordination of these efforts must cross budget lines as well as spheres of interest and academic training.

A third barrier arises between researcher or modeler and the user of the model. The user (e.g., in Washington, D.C.) is often physically removed from the modeler (in EPA or contractor laboratories) and may not be scientifically trained; it may be difficult to communicate what is desired from the model and what can reasonably be expected.

The modeler may also be separated from the user by attitudes and objectives. A decision-maker evaluates a particular model to be used for predictive purposes, in terms of its applicability, accuracy, availability of input data, comprehensibility and cost. The research scientist, on the other hand, is less interested in prediction than in furthering his understanding of the process or system being modeled. Thus, the scientist's criteria for evaluating the usefulness of a model as a research tool would include:

- theoretical foundation
- accuracy and validation
- availability of data inputs.

He would be less interested in its applicability, comprehensibility and cost. Both parties must communicate their objectives explicitly and try to understand the capability of the model in relation to these different objectives.

It should also be noted that much work in this area is being conducted by academic and private research institutions, where the publication of new findings is important to individual success. This provides an incentive to regard planned research as proprietary rather than as information to be shared.

The imbalance of research effort noted above is in part a result of these barriers. Moreover, available models appear often to have been developed as a by-product of research for other purposes. Consequently, they are fragmentary and frequently are not followed through to the application stage.

SECTION III

RECOMMENDATIONS

The following recommendations concern the process by which models are developed. Because exposure assessment modeling is still not operational and because there is no consensus on what approaches are likely to be most effective, specific recommendations for marginal changes in existing models are not appropriate at this stage. Instead, the recommendations focus on steps that could be taken to establish priorities for a research effort in this area.

1. Statistical studies of factors affecting population exposure should be conducted. The resulting data would be a vital link in exposure assessment modeling and would advance the understanding of which parameters may be significant for estimating human behavior.
2. A careful, published record of environmental conditions prevailing in experimental or field studies should be required. A comparison of such records would provide clues to possible synergistic or antagonistic effects.
3. All models should explicitly consider input data needs and the feasibility of collection. For the environmental fate models the emissions data were most often cited as inadequate. Because of the importance of such factors as control equipment, quality of maintenance and age, an emissions inventory should be based on observation of actual sources rather than engineering estimates. The current lack of technology to detect low concentrations of many substances in the environment may be a limiting factor for this type of modeling.
4. In order to improve communication between modeler and user, meetings should be held which both research scientists and policy makers attend. These meetings should cover both the needs of the decision-maker and the capability of the models.
5. Improved reports describing the models are needed to facilitate communication among scientists and between scientists and users. Because no consensus exists on how to do an exposure assessment, a rapid dissemination of technical information is required. It would be helpful if every EPA

report of a research effort involving modeling were required to include information on:

- input data required and how obtained
- theory and assumptions employed in the model
- output produced, its form and estimate of accuracy
- sensitivity analysis results for key parameters
- applications and validations attempted
- cost
- documentation on how to use.

Several points in this list deserve emphasis. It is important to report gaps in the knowledge or assumptions made. Modeling is an excellent way to discover such gaps but the need to complete a model also serves to cover over those gaps. To the user who must choose between alternative models, cost estimates can be as important as output results.

6. Reports should be made for studies producing non-results. It is understandable that research scientists find little stimulation in conducting and documenting exposure studies at concentrations or for substances that fail to produce changes in the biologic system in which they are interested. The conduct and reporting of such studies, however, is important for a total evaluation of risk. Knowledge of non-results would assist in making trade-off decisions because the lack of risk as well as benefit is an important factor in such decisions.

SECTION IV

MODELING EXPOSURE AND EFFECTS

Quantitative exposure assessment involves estimates of the size of the exposed population, the concentration level and duration to which it is exposed, and the effects expected to result from this exposure. The following sections present an account of techniques by which exposure and effects can be estimated for humans, a review of ecological modeling of plant and animal populations, and a discussion of the few studies done to estimate the size of the exposed population.

HEALTH EFFECTS

Exposure assessment modeling attempts to infer dose-response relationships relating health effects to the level and duration of exposure to the potentially toxic substance. Much of the research being done in this field is directed toward developing relatively quick and inexpensive tests that can be used to screen substances for potential toxic effects. For example, under the Toxic Substances Control Act of 1976 a hierarchy of tests is likely to be required in determining whether a new chemical can be produced. Such tests by themselves may not yield the information necessary to establish a dose-response relationship because the focus is on the effect and doses may not vary. Some difficulties with this and other approaches to measuring health effects are discussed below.

Several problems confront the researcher attempting to establish a dose-response. The health effect of a single exposure or repeated short-term exposures may--or may not--be different from the effect of long-term low-level exposure. Acute adverse effects may be the cumulative result of long-term lower-level exposures, or the effect of short-term peak exposures. Conversely, chronic effects may follow short-term peak exposures, as well as long-term low level exposures. In general, it is easiest to obtain data on acute effects following short-term exposures. Less information is available on acute and chronic effects following long-term exposures and very little is known about measuring chronic effects of peak exposure.

Another complication is the possibility of synergism or

interactions between substances in producing effects. When studies are limited to a single pollutant or chemical, the effects produced may not be representative of actual environmental conditions. Another substance not present in the laboratory situation may enhance or inhibit the effect in the real world.

A third problem is extrapolation. Tests made on animals may not be applicable to humans because the animal may metabolize the substance differently or because the animal's organs may be differentially sensitive to the substance. The interpretation of tests involving atypical levels of exposure is also problematic. Often a testing procedure will use high levels of the substance over a short period of time in order to produce a measurable effect and lower the cost of the test. These levels and durations may not correspond to any actually observed in the environment; the problem is how to use such a test to predict effects at low environmental levels. This problem will be more fully discussed in the next section of the report.

The problem of determining dose-response relationships has been attacked through epidemiology, clinical research and animal toxicology. Each of these approaches suffers to some extent from the difficulties described above.

Epidemiological studies are set in the real world and allow consideration of the effect of long- and short-term pollutant exposures on different groups of the human population. Often, however, only crude measurements of health effects are possible; in addition, such studies frequently cannot adequately control for all influencing factors and are restricted to a limited range of exposures.

More sophisticated health measurements and controlled exposures are possible in clinical studies. Human studies, although expensive, have the obvious advantage of eliminating the need to extrapolate the results from another species to man. However, long-term exposures cannot be easily evaluated.

Toxicological testing provides an opportunity for carefully controlled studies that may involve a wide range of pollutants and actual examination of affected body tissues. These tests often serve largely as the basis for judging whether the exposure of a living system to a chemical presents a hazard. However, differences among species and between animals and humans limit the usefulness of such studies. This approach is quite costly for tests of chronic effects.

Given their various imperfections, it may be appropriate to use all three approaches for a particular problem. The studies should be designed to complement each other and to elucidate the biological mechanisms involved. Finklea's review

(1977) of available research on exposures to certain air pollutants shows that there has been an imbalance between the three research approaches as well as a lack of quantitative data about several effects of major concern. Atkeson (1976) attributes this problem in part to the lack of effective coordination of research on effects. Similar conclusions are summarized in an EPA report (1978) on health effects of transportation-related pollutants. Information on what research is planned or in progress is not easily available, especially outside government agencies. Also, because there is little interaction between health scientists and modelers of transport and transformation of pollutants, independent researchers may establish priorities that greater shared understanding would show to be inappropriate; duplication of effort is also a problem, and there is the danger of overlooking a potential health hazard.

DOSE-RESPONSE RELATIONSHIPS

To estimate the health consequences of changes in environmental quality, a dose-response relationship must be established. Several difficulties may arise. There is little biological theory on how a substance affects the body. In the field of pharmacokinetics, the metabolic model (Friberg, 1976) describes processes of absorption, distribution, deposition, etc. at the cell and organ level in order to estimate the critical concentration or threshold level at which an effect is produced. This procedure is potentially applicable to effects resulting from long-term exposure to a substance with a long biological half-life, but it requires an enormous amount of information, little of which is currently available.

A more commonly used approach is to do animal experiments or occupational exposure studies. However, the data collected in such exercises may not be suitable for establishing a dose-response relationship. An effect may be recorded and described as to degree of severity. For a given population and given dose the measure reported as effect is percentage showing the effect. A different measure is response. Response enumerates "reactors," percentage of the population all given the same dose and exhibiting the same effect. Examples are LD_{50} or LC_{50} , common statistics collected in toxicity studies. The statistic LD_{50} is the dose causing death of 50% of the population; LC_{50} is the concentration causing 50% of the population to show the given effect. Unfortunately, the tests may be conducted in such a way that it is not possible to separate the two measures--effect and response. The results may be due to both an increase in the severity of the effect and an increase in response for each effect as the exposure level increases.

Second, the commonly accepted concept of "dosage" may obscure some important differences. Dosage is defined as the

product of concentration level and exposure duration or time. But equal dosages may not produce equal effects. Larsen (1977) has shown that concentration is more important than exposure duration in causing excess mortality in mice exposed to nitrogen dioxide. This problem can be overcome, but it is often important to give separate attention to the two factors of concentration and duration when reporting and using experimental results.

Third, even when experiments are carefully conducted and reported for the specific purpose of establishing dose-response relationships, it is usually necessary to extrapolate from the results to the much lower doses encountered in the environment. Several approaches are taken in the literature. One is to assume there is a threshold, a definable concentration below which a chemical will not produce a toxic response in an exposed subject. However, this assumption solves the problem of extrapolation only if a study has been done at low enough concentrations that no effects are observed. EPA's National Ambient Air Quality Standards are an example of the use of thresholds.

Another approach is a straight-line projection from the experimental result to zero dose, which assumes there is no threshold or safe level. This is called the linear or "one-hit" model, since it assumes that each increment of exposure has the same independent low probability of causing the effect, regardless of the dosage level. This assumption is generally accepted for radiation studies. However, such a model is not likely to be realistic for chemicals, but rather would define only an upper limit to the level of effects likely at very low doses. Because physiological detoxification mechanisms would render small doses less effective, there would probably be some sort of threshold or at least a smaller effect per dose increment at low levels.

A third approach, the log-probit model, is based on the assumption that the observed changes in response are the result of variations of susceptibility in the population. This variation is assumed to be log-normally distributed with dose. This approach has been followed by Larsen (1976 and 1977) in assessing both plant injury and animal mortality. It is based on the finding by toxicologists and pharmacologists that an organism's response to a drug dose is often proportional to the logarithm, rather than the arithmetic value, of the dose. They have also found that there is a range of doses so low that no response is measured, and a maximum response that will not be exceeded even if the dose is increased. Such data thus appear to be log-normally distributed. The major problem with this model is that the normal distribution may not be as reliable in the tails of the distribution as in the central part. Unfortunately, it is precisely the tails (very low environmental exposures or high accidental exposures) in which we are interested and the

probit function obtained from the observable range may overestimate the probability of a response at low doses.

A final recently suggested approach is based on kinetics (Cornfield, 1977). It assumes a reaction in which the toxic substance is deactivated by another substance, but which may be reversed, disassociating back into toxic agent and deactivating agent. This model produces a dose-response curve shaped like a hockey stick, flat up to the threshold level and rising steeply afterwards, once the protective or deactivating mechanisms are saturated. The existence of such a threshold level depends on the existence of at least one protective reaction.

Cornfield (1977) provides a good survey of the various approaches to estimating dose-response relationships. All of these approaches are still largely conjectural and much remains to be learned from experimental tests for a wide range of dosages.

ECOLOGICAL MODELING

Because direct experiments can be made on plants and animals, there should theoretically be no need to extrapolate from one species to another. However, in practice such experiments are exceedingly expensive and choices must be made about which studies to conduct and how to extrapolate from them. Models of the processes of interaction of plants, animals and the environment would aid in making these choices. Until recently, however, ecologists have focused on qualitative descriptions of the structure and dynamics of relatively undisturbed ecosystems. It is only in the past decade that modeling has played an important role in ecological research. Modeling can enhance fundamental understanding by organizing the research effort, synthesizing existing knowledge, analyzing hypotheses about a system's structure and dynamics, and identifying fundamental constraints on a system's functioning and the mechanisms to which a system's behavior is most sensitive. As a predictive or management tool, modeling can also be used to measure environmental changes caused by human-induced disturbances of natural ecosystems.

Management models include models of terrestrial grazing systems, fisheries and pest control. These models have foundations in population dynamics including basic processes of predation, competition, birth, death and migration. To model environmental factors, the concepts of flow, threshold and interference must be included. The flow of materials or energy between populations reflects the dynamics of interacting populations and feedback mechanisms that occur in nature. Threshold effects include the appearance of behavioral or physiological responses that would substantially alter the form of the rela-

tionship between the population and its environment. Interference may be due to the scarcity of material resources as opposed to the effects of direct competition for available space. The few working models of the management type are summarized in Wiegert (1975). In general they are confined to a single species or link in the food chain and do not incorporate feedback or threshold effects. Wiegert (in press) has proposed a method for incorporating these effects but the applications remain limited to single species.

Ecosystem models, which include more than a few component species or environmental conditions, are primarily directed toward an understanding of the natural system and the identification of critical parameters and processes. These include models dealing with aquatic ecosystems, forest, grassland, tundra, desert and soil-litter. They focus on the integrated dynamics of the entire community under study and describe the flow of energy, biomass, and nutrients through the system. Aquatic ecosystem models are probably the most numerous and have grown out of a desire to simulate water quality changes as well as quantities and flow. Patten (1976) presents some of the more recent of these models which describe both aquatic and terrestrial ecosystems.

Ecosystem models must relate physical, chemical and biological processes. Although considerable progress has been made in developing realistic mathematical models such as these, several remaining major problems limit their predictive ability. These problems include the requirement of a multi-disciplinary approach, sparse data sets, biological variability, interactions of processes operating at significantly different temporal and spatial scales, and nonlinearity.

Because many disciplines are involved, most modeling efforts require a team approach. There has not been a great deal of experience in organizing and maintaining modeling teams. Nor have fundamental unifying theories been developed that can be used to deduce quantitative ecological behavior. Thus, existing models often reflect the expertise of their builders in being sophisticated in one respect and quite crude in others.

The lack of a unifying theory may also exacerbate the problem of data availability. Many data sets exist for a given phenomenon or system but few contain measurements of all the factors that are important in controlling the dynamics. Different parameters observed in nature may be indicators of the same substances; some indicators may be redundant. It may be difficult to apply a model because the data needed to quantify all the model's parameters may not be available for a specific situation. On the other hand, not all the substances that have been quantified by analysts are of real ecological significance. The problem is to select a set of both meaningful and measurable

parameters that will reflect sufficiently the ecological changes of interest. It should be noted that collecting the data needed to estimate the parameters or validate an ecological model usually takes a long time.

Biological variability or uncontrolled factors make ecosystems much more difficult to model than physical transport systems. Not all individuals of a species placed in identical environments will respond identically, due to differences in heredity and/or environmental preconditioning. This variability poses special problems for deterministic models and may argue for the incorporation of probabilistic elements.

The interactions between the various components of an ecosystem are played out over an extremely broad temporal and spatial range. Actions and reactions are delayed in time and components are nonrandomly arranged in space. One solution is to run many concurrent models, each appropriate to a given spatial-time resolution. However, the problem remains if the areas being modeled change in size or the spatial heterogeneity itself changes over time.

Ecological phenomena are inherently nonlinear. Both threshold and saturation reactions occur commonly in ecological systems. Nonlinear interactions make mathematical analysis of a model complex.

A large body of mathematical theory is concerned with deriving analytical solutions to linear systems; this work gives insight into the functioning of a system and can be used to check the model for logical or conceptual inconsistencies. The argument for the use of linear equations as a reasonable approximation is that behavior is linear if the state variables fluctuate around some given point, such as an equilibrium point. However, linear equations can only show how the system operates, not why it operates as it does. If wide fluctuations or changes in policies occur, more realistic nonlinear equations may be needed. In addition, the use of nonlinear interactions may increase the stability of a system simplifying the system's response to the disturbance. Further discussion of this problem is found in Bledsoe (1976).

It should be noted that the scope of this report has prompted a somewhat narrow view of ecological modeling. Much work is being done with physical models of systems in the form of microcosms in the laboratory. They provide an overall assessment of the complex interactions taking place but are not a mathematical model in the sense we use the term in this report.

HUMAN POPULATION EXPOSURE

The main environmental routes through which humans are exposed to pollutants are air, water, and food. Human behavior patterns as well as pollutant characteristics will determine which of these routes are important avenues of exposure. Transport and transformation models predict concentration levels in the various media on the basis of the specific characteristics of the substance. In making an exposure assessment it is also necessary to estimate the size of the population actually exposed to these concentrations.

Air

Studies of air pollutants have generally estimated population exposure from census data by determining how many people live within a certain radius of the sources (Kuzmack and McGaughey, 1976 and Mara and Lee, 1977). Several problems are inherent in such a methodology. Census data concern residents of an area, but people spend part of their time away from home. If the substance is a localized air pollution problem, travel patterns would affect exposure. Generally no allowance is made for this. However, Horie and Stern (1976) have done an analysis for the sub-populations of school-age and elderly (as well as for the whole population), eliminating the working-age population because of its greater daily mobility.

In addition, the length of time a person lives in the area will be important. Thus, some account should be taken of longer-term mobility into and out of the area. Horie and Stern (1976) correlate ambient air concentrations for each year with the census data for that year. EPA (1977) has incorporated this factor by using an average figure for the entire U.S. (6.7 percent of U.S. population moves out-of-county each year).

These methods yield an estimate of a level of concentration that is assumed to be continuous. However, health effects may vary according to duration as well as level of exposure. Horie and Stern (1976) have estimated various long-term and short-term exposures to obtain measures of population-at-risk, the distribution of population associated with various dose levels above the EPA standards.

Another problem in using census data is matching the location of sources and concentration levels or air monitoring stations with census statistical areas on a geographical basis. Mara and Lee (1977) assume the source is at the city center and use the population density for that city. EPA (1977) assumes average population densities for urban areas. Horie and Stern (1976) aggregate the population data to establish points within an area indicating resident population and then interpolate air

quality data from air quality monitoring stations nearest the point.

Water

The other routes of exposure are even less well described than air. Generally, if the source of a pollutant is drinking water, some average intake of water per day is assumed, with the average concentration in water determined through tests.

Food

Reliable estimates of exposure through food are especially difficult to obtain. It is difficult in any case to analyze the substances in food; in addition, the analysis is often done on raw food whereas the actual exposure takes place through a mixed diet or processed foods. Concentrations of the substance in question may increase or decrease during processing. Thus, assumptions about the types, the amounts and the processing of food must be made.

Occupational Studies

Environmental exposures are not the only source of contact with pollutants. Indeed, exposure at the workplace can be a dominant source for some substances. Occupational studies generally take the form of surveys of effects and exposure levels. Because it is possible to link exposure and effect more directly than in environmental studies, occupational investigations can provide a more accurate estimate of risk. However, because the concentration levels are generally much higher than environmental exposures, findings are not directly applicable to those not occupationally exposed. This problem was discussed in the sections on health effects and dose-response relationships.

SUMMARY

Table I summarizes the broad areas of exposure and effects modeling according to the decision-maker's criteria presented in the introduction to this report. Generally, health effects are not modeled but are obtained from laboratory or field experiments. Very little sensitivity analysis or cost information is provided in any of the areas. The human exposure models have not been well validated; moreover, data availability problems often permit only highly aggregated estimates. Ecological modeling is still very much a developing rather than an operational endeavor.

TABLE I

EVALUATION OF EXPOSURE AND EFFECTS MODELS

Type of Model	Applicability	Accuracy, Validation	Input Data Available	Assumptions	Sensitivity Analysis	Cost
Health Effects Studies	Output units vary widely, making it difficult to combine studies. Methods applicable to many types of pollutants.	Confidence limits often established. Comparisons between studies sometimes done.	Not in model form so not require input data.	Initial conditions and other factors not always reported.	Not usually done.	Varies but not usually reported.
Eco-logical Modeling	Output units and species included vary widely.	Usually not known.	Require large amount of site specific data.	Initial conditions not always reported.	Not usually done.	Not reported.
Human Population Exposure Studies	Output relevant though highly aggregated.	Not known.	Census data most often used.	Explained.	Not done.	Not reported.

SECTION V

MODELING INTERFACES BETWEEN MEDIA

Models of the environmental fate of substances and of their transport are used to predict pollutant concentration--a necessary input to the exposure and effects models discussed earlier. Although relatively advanced, the fate and transport models typically consider only a single pollutant and a single medium of transport.

Assessing the single medium fate and transport models of air and water quality is beyond the scope of this report. Briefly, however, models of urban scale (50 km) are the most advanced of the air quality models. They model the dispersion process for area and point sources and for reactive and un-reactive gases. Some allow for variations in meteorology; most are limited to non-complex terrain. These models are now being validated with field data, and efforts are being made to simplify the required data input, depending on the application, and to assess the models' accuracy and costs. This work is being done at the EPA Environmental Sciences Research Laboratory, Research Triangle Park, North Carolina.

Research has also begun on microscale (0 to 500 meters) and regional scale models. Regional scale models must incorporate sink processes and chemical transformations that do not appear for the urban scale.

Water quality models exist to model transport and transformation of substances from point discharges and non-point sources, including urban and non-urban runoff. The process rates differ according to the type of water body (lake, river, estuary). Most of these models incorporate a mass balance equation describing flow into and out of a given section of water. Processes such as chemical and biological transformations are accounted for as sink processes whose rate constants are estimated from empirical data specific to the site being modeled. The models predict concentration levels for water quality parameters such as dissolved oxygen, nitrogen and phosphorus compounds. More recent models incorporate heavy metal transport and pesticide dispersion.

The air and water quality models were developed in response

to a perceived need to control direct emissions or discharges. However, a source of contamination can also be indirect, as in an intermedia transfer. Thus, our investigation focused on how to model these intermedia fluxes in order to predict concentrations in all media of the environment. This report describes models that simulate the processes at the interfaces, including:

- for the air and water/soil interface
 - wet deposition
 - dry deposition
 - evaporation or volatilization
- for the soil and water interface
 - adsorption-desorption
 - transport from soil to aquatic system (infiltration and run-off)
- uptake by biological systems

AIR AND SOIL/WATER INTERFACE

Pollutants emitted directly into the atmosphere are dispersed through space over time. There are air quality models that describe this process and estimate pollutant concentrations in space and time as a function of the emissions distribution and certain meteorological and geographic conditions. In addition to the dispersion process there are sink mechanisms which serve to remove the pollutant from the atmosphere altogether. These removal processes include:

- 1) chemical reactions or transformations
- 2) gravitational sedimentation (for particles with radii greater than 5-10 μm)
- 3) wet deposition
 - a) rainout (pollutant first absorbed by cloud then brought to ground by rain)
 - b) washout (pollutants collected by falling raindrops)
- 4) dry deposition (impingement of particles onto elements of earth's surface as well as absorption of gaseous compounds)

Because the residence time of most pollutants is much longer than the time it takes for winds to carry the pollutants out of the local area under consideration, the effect of sink mechanisms has not been included when modeling air quality on an urban scale. Recent efforts to improve air quality models and extend them to a regional scale (100 to 1000 km) have concentrated on including the transformation and deposition processes, since sedimentation is negligible for gases and most traces metals are emitted as air pollutants.

At the interface between air and water or land it is the deposition process which is at work. Several models now being developed include deposition.

Source Depletion Model

The atmospheric dispersion process can be described by a Gaussian plume model for a non-depositing material assuming 'reflection' of the material at the ground to insure conservation of mass. A source depletion model can account for the loss of airborne material due to deposition by reducing the source strength as a function of downwind distance. The deposition of airborne material is a little understood physical and chemical phenomenon. In the absence of detailed microphysical measurements, Chamberlain (1960) suggested the use of the concepts of washout ratio and deposition velocity.

The washout ratio, W , is the ratio of the concentration of the pollutant in air per kilogram of air and its concentration in rain per kilogram of rain. C The amount of deposition per unit area, D_w , is taken as $D_w = W \frac{C}{P} R$, where C is the concentration of the pollutant in air, P is the density of air and R is rainfall. Thus, wet deposition is assumed to be proportional to the local air concentration for a given amount of rainfall. Generally, washout ratios must be measured at the site in question. Some representative washout ratios as a function of particle size can be found in Gatz (1975).

Similarly, the rate of dry deposition per unit area (D_d), is usually assumed to be directly proportional to the local air concentration (C) evaluated at a reference height:

$$D_d = V_d C$$

The constant of proportionality V_d has the dimensions of velocity and has been named the deposition velocity. Several theoretical models have been developed to predict the exchange rate (or deposition velocity) of gases at the air-water interface and will be discussed below. However, measurements of the deposition velocity are generally required. Gatz (1975) presents deposition velocities for many trace metals as a function of particle size. Prahm et al. (1976) summarizes the various measurements taken of the deposition velocity for sulphur dioxide.

Several aspects of this interface problem have been examined in more detail. These include the mechanism (source or surface depletion) used to deplete the Gaussian plume, refinements of the deposition rates to allow for dependence on factors other than concentration, and attempts to model plant uptake or the actual mechanisms involved in the deposition process.

Surface Depletion Model

As described above, the source depletion model reduces the source strength according to the air concentration at a given distance downwind. The reduction is in effect instantaneously

distributed throughout the vertical extent of the plume. This produces an artificial vertical mixing of the plume. A more realistic model has been developed which selectively depletes the Gaussian plume in the vicinity of the deposition surface (Horst, 1977). This surface depletion model allows deposition only from the lowest layer, eliminating the artificial mixing of the source depletion model. It predicts longer residence times for airborne materials. This can be seen from the equations used in the different models.

$$\text{Source depletion: } C(x,z) = [Q_0 - \int_0^x v_d C(x',z_d) dx'] \frac{D}{u}(x,z,h)$$

Surface depletion:

$$C(x,z) = Q_0 \frac{D}{u}(x,z,h) - \int_0^x \frac{v_d}{u} C(x',z_d) D(x-x',z,0) dx'$$

where C is the concentration at a distance downwind (x) and at a height (z), Q_0 is the source strength, h is the source height, z_d is the reference height near the surface, u is the wind speed, v_d is the constant of proportionality with the dimensions of velocity, and D is the diffusion function with the dimensions of reciprocal length. Comparing the variables upon which D is functionally dependent shows that the source depletion model assumes deposition is a loss at the source rather than at the surface.

The source depletion model overpredicts the surface air concentration and deposition close to a source and overestimates total deposition between source and receptor. However, the surface depletion model is computationally more complex. Horst (1977) presents quantitative comparisons to aid in the choice between the two methods.

Recently, in order to incorporate information on the vertical mixing process (atmospheric stability), a finite difference box model was developed (Draxler and Elliott, 1977). The model is Lagrangian in character since the deposition is computed along a path rather than at a particular location. Discrepancies similar to those presented by Horst (1977) were found between the source depletion and the surface depletion methods. The purpose of the model, however, was to test the impact of atmospheric stability on deposition rates. Using hypothetical data, it was found that atmospheric stability at the time of emission release was one of the primary factors determining the pollutant's residence time in the air.

Wet Deposition Rates

The application of the washout ratio described earlier de-

pendent on knowing the total rainfall occurring over the modeled region and assumed it fell at a steady, uniform rate. Another approach is assuming that the onset of a wet (or dry) period occurs with a constant transition probability and to include the washout ratio function only during a period of rainfall. This method, proposed by Rodhe and Grandell (1972) and employed by Fisher (1975), uses the same washout ratio but requires information on the mean lengths of wet and dry periods. A sensitivity analysis by Bolin and Persson (1975) shows that when a smaller value for the washout ratio is chosen, the deposition due to rainfall becomes more evenly distributed over a larger area.

Dry Deposition Rates

Using a constant value for the deposition velocity ignores the dependency of deposition velocity on the height above the surface, various surface characteristics and atmospheric conditions. However, if a representative value for the deposition velocity could be determined, the long-range transport models described above could predict the rate of deposition solely by predicting a surface layer concentration for the pollutant. For particles, measurements have been taken to relate deposition velocity to particle size (Gatz, 1975) and to particle size and wind speed (Winchester and Duce, 1977).

For gases, models have been developed to estimate deposition rates using theoretical considerations and laboratory and field measurements. They predict the rate of transport from the air to both water and land surfaces (vegetation) and evaluate some of the factors affecting deposition rates (Wesley and Hicks, 1977; Bennett et al., 1973; O'Dell et al., 1977; Shreffler, 1976). These studies are still limited and in the development stage. Generally, they model mass transfer at the microphysical stage using a series of resistances analogous to electrical resistance (Spedding, 1977). A description of these studies can be found in Table II.

Evaporation or Volatilization Rates

The deposition models we have been discussing are steady-state models, requiring that the flux of the gas across both boundary layers (e.g., from air to water and from water to air) be constant. Thus work in this area has applications for the measurement of evaporation rates as well as deposition rates.

The process by which a compound is transferred from soil or vegetation to air is called volatilization and is modeled in the same way as evaporation. For high-solubility and/or high-reactivity substances such as SO_2 , the models predict deposition rates and the water or vegetation acts as a sink. For low-solubility compounds, such as pesticides, the models predict evaporation or volatilization rates from water or land to air.

TABLE II
STUDIES OF DEPOSITION AND EVAPORATION RATES

Reference	Substance	Canopy Type	Model Type	Input Data	Results
Whelpdale and Shaw (1974)	SO ₂ (deposition)	grass snow water	bulk transfer analogues to water vapor	bulk transfer coefficient of water vapor, average wind speed, concentration gradient	$V_d = 5$ to 2.5 cm/sec, greatest over water, least over snow, decrease with increasing atmospheric stability
Liss and Slater (1974)	gases (evaporation)	water	two-film resistance model	empirical estimates of atmospheric transfer coefficients	rate for low (high) solubility gases liquid (vapor) phase controlled
Mackay and Leinonen (1975)	Low solubility gases (evaporation)	water	resistance model	lab measurements of mass transfer coefficients and Henry's Law constants	rate is liquid (gas) phase controlled if vapor pressure to solubility ratio high (low); rate sensitive to temperature only if vapor phase controlled
Hicks and Liss (1976)	SO ₂ and other reactive gases (deposition)	water	model of flow-gradient relationship	empirical estimates of relationships	calculates V_d as function of wind speed, atmospheric stability and height of observation
Smith et al. (1977)	Soluble organic substances (volatilization)	water	two-film resistance model	molecular diameter of substance, oxygen reaeration rate	volatilization rate constant

TABLE II - continued

Reference	Substance	Canopy Type	Model Type	Input Data	Results
Farmer and Letey (1974)	Pesticides (Volatilization)	Soil	diffusion and mass flow equations	vapor pressure of pesticide, temperature & wind speed	volatilization rate
O'Dell et al. (1977)	Gases (deposition)	Vegetation	resistance model	aerodynamic, stomatal and mesophyllic resistances	at high wind speeds aerodynamic resistance negligible; for highly soluble gases mesophyllic resistance negligible
Wesley and Hicks (1977)	SO ₂ and similar gases (deposition)	vegetation (dense uniform)	resistance model	aerodynamic, surface and canopy stomatal resistances	V _g as function of height of observation, wind speed, roughness length, canopy stomatal resistance and Henry's Law constant
Slinn (1977)	Particles and gases (deposition)	water and vegetation	semi-empirical formulas for wet and dry deposition	much input data required but not available	deposition of gases dictated by other than atmospheric processes
Shreffler (1976) Viebrock (1977)	Gases (deposition)	vegetation	resistance model	stomatal and aerodynamic resistances, surface concentration	flux depends on height, zero-plane displacement, roughness, leaf area density
Neely (1977)	Chemicals	water	based on results from Liss and Slater, Mackay and Leinonen	molecular weight, temperature, solubility, pressure	formula for evaporation rate constant

These models require measurement of such basic variables as roughness, length, wind speed, canopy resistance, and Henry's Law constant, among others. The values of these properties, however, are rarely available for a large area. Precise values are usually only obtained by micro-meteorological experiments. On the macroscale, flux can be calculated directly from field measurements and deposition velocity estimated from flux and concentration values. The usefulness of these models lies in the possibility of deriving generalizations about the likely values of deposition velocity and the way various factors might affect it.

Wesley and Hicks (1977) outline one procedure that could be used in the case of a regional-scale model of SO_2 or other highly soluble gases. They include factors for atmospheric stability, surface roughness (type of vegetation) and wetness of exposed surfaces (crop moisture index). These values, though imprecise, could be obtained from available resources and might suffice in view of the large inaccuracies resulting from other assumptions in such a regional model.

SOIL AND WATER INTERFACE

Pollutants deposited on the land, like those emitted to the air, are subject to transformation and transport, though the processes may differ. The following processes are known to influence the fate and behavior of pollutants in soil systems:

- 1) microbiological and chemical reactions (degradation)
- 2) adsorption-desorption
- 3) volatilization
- 4) movement or transport (infiltration, run-off)
- 5) plant or organism uptake

The last four processes, of course, affect both the original compounds and the products of the degradation process.

Most studies of these processes have been concerned with the transport and fate of pesticides or other organic compounds. The following discussion will rely heavily on the organic compounds literature.

Volatilization was discussed in the previous section and is the major transfer process at the air-soil interface. The phenomenon of adsorption-desorption directly or indirectly influences the magnitude of the effect of the other processes. It appears to be a major factor affecting the interactions of pollutant and soil and transfers across the soil-water interface. We will now describe the way pesticide transport models incorporate the adsorption process.

Adsorption-desorption

Adsorption is the attraction of pollutant molecules to soil particles; the reverse process is known as desorption. How much of an available substance is adsorbed determines how much can be transported in solution and in sediment from the soil to the water phase of a system. A number of factors determine the extent of pesticide adsorption in a soil-water system. Generally, these are related to (1) the nature of the soil, (2) the nature of the pesticide, and (3) the influence of environmental conditions. Bailey and White (1970) and Browman and Chesters (1977) have summarized current understanding and research on these factors.

Because quantitative relationships describing the effects of these factors on adsorption have not been developed, pesticide transport models use empirically derived equations relating equilibrium solution concentration to the amount adsorbed. Several adsorption equations have been proposed and are described by Bailey and White (1970) and by Browman and Chesters (1977). The Freundlich equation is the one most frequently applied to natural systems and takes the form $\frac{x}{m} = KC^{1/n}$ where $\frac{x}{m}$ is the amount adsorbed per unit soil, C is the equilibrium concentration in solution and K and n are empirically derived constants. This describes an equilibrium state and assumes the process is reversible.

It has been shown that some pesticides are so strongly adsorbed that not all of them will desorb. Even under repeated washings some portion will remain permanently fixed or adsorbed. Crawford and Donigian (1973) have developed a model to account for this irreversible adsorption. Their adsorption equation is $\frac{x}{m} = KC^{1/n} + \frac{F}{m}$ where F/m is an empirical term for the amount of the pesticide adsorbed in a permanent fixed state. This term, F/m, is less than or equal to the permanent fixed capacity of the soil for that pesticide. This maximum capacity is approximated by the cation or anion exchange capacity for the particular soil type. All available dissolved pesticide is assumed to be adsorbed into the permanent fixed state until the maximum is reached. The remaining dissolved pesticide is then subject to reversible equilibrium adsorption according to the Freundlich term, $KC^{1/n}$.

This model assumes, therefore, that reversible adsorption is single-valued. Research has indicated that this assumption is not valid for many pesticides. Tests of this model have shown that it did not adequately simulate the division of pesticides between the sediment and solution phases. This was especially true for soluble pesticides which also adsorb onto soil particles.

A newer model by Donigian and Crawford (1976) allows for

non-single-valued-adsorption/desorption. In this model the desorption equation is $x/m = K'C^{1/n} + F/m$. The user must specify n' and the model calculates K' as a function of K , n and n' , the other adsorption/desorption parameters. Comparison of simulation results from single-valued and non-single-valued adsorption/desorption functions with observed data is inconclusive. One form performs better for some storms, while the other form performs better for other storms (Donigian et al., 1977).

So far we have been concerned with soil-pesticide interactions at the soil-water interface. Adsorption also governs sediment-pesticide interactions at the sediment-water interface. However, in this case adsorption will depend on different factors, such as particulate matter already present in the aquatic system, the aerobic-anaerobic cycle, and the degree of mixing that occurs. However, since the mechanisms underlying the adsorption process have not been modeled, the Freundlich equation and its empirically estimated constants are also used in the case of sediment.

Transport from Soil to Aquatic Systems

During precipitation pollutant residues can be transported vertically through the soil (infiltration) into the groundwater or across the soil surface (runoff and sediment loss) into rivers or lakes. Usually models represent infiltration by a capacity curve in which the capacity is an exponential function of time. This assumes that the supply rate (precipitation minus interception plus surface detention) always exceeds capacity. When this is not the case, variation in infiltration capacity is controlled by accumulation of soil moisture as well as time. Crawford and Donigian (1973) describe infiltration equations that can be used to relate infiltration capacity to soil properties and time but are still based on empirical estimation of the soil parameters. They also apply the method so as to account for variations in soil properties throughout the watershed modeled.

A considerable number of hydrologic models have been developed to simulate runoff. The more recent ones include the infiltration process. Generally, they are intended for application either in rural areas (e.g., non-point source pollution from agricultural lands) or urban situations (e.g., stormwater runoff to sewer systems). A description of these models will not be attempted here since they vary widely in scope and purpose, mathematical detail, data requirements and computer output. Several papers have reviewed the various models. Perez et al. (1974) gives a summary of runoff and groundwater models. Brandstetter et al. (1976) reviews urban runoff models. Donigian and Crawford (1976) describe an agricultural model of pesticide transport.

Our descriptions of the adsorption, infiltration and runoff processes have been derived mainly from models concerned with pesticides or organic compounds. Because these processes are largely described by empirically determined relationships, similar models are applied to heavy metals. One example is the Unified Transport Model (Van Hook and Shults, 1976). In this model experimentally determined solubility constants form the basis for estimating losses from litter to infiltration and surface runoff. Once within a soil layer, exchange of the heavy metal is assumed to take place instantaneously and the amount exchanged depends on a measured distribution coefficient. The use of cation exchange capacity to describe adsorption, however, is not universally recognized as the dominant process in environmental fixation of trace metals. Some researchers propose instead that hydrous oxides of iron and manganese may control the exchange process (Korte et al., 1976). Thus, as in the case of pesticides, the process of adsorption is not well understood and may not be well described in current models.

UPTAKE IN BIOLOGICAL SYSTEMS

Plants absorb gaseous pollutants and the process (deposition) has been modeled as a series of resistances to transfer across the air boundary layer over the surface of the leaf. The absorption process from soil and water is usually described by the use of partition coefficients (concentration in organism/concentration in soil or water) comparing distribution of the chemical in one phase to that in another phase.

Such coefficients do not represent absolute distribution coefficients actually occurring in nature since these are governed by an enormous range of factors. Even as a relative measure of distribution they are at best indicators of pollutant behavior rather than precise tools for prediction.

How a compound partitions between water and hydrocarbon-containing organisms such as aquatic plants and animals is apparently related to whether it is polar (as judged by its water solubility) or non-polar (as judged by its fat solubility). The partition coefficient of the substance between octanol (a compound midway in the range of fat/water solubilities) and water is sometimes used as a predictor of relative partition coefficients. Neely (1977) uses this method. If the octanol/water partition coefficient is unknown, it is estimated from the solubility.

Several methods for estimating the absolute value for uptake of chemicals by plants and fish have been suggested. Metcalf (1977) uses the pharmacokinetics of drug absorption and metabolism to express the concentration rate as a function of concentration in water, absorption rate determined by the lipid/

water partition coefficient, organism mass or volume and the rate constant for clearance of the drug by the combination of the processes of degradation, elimination and growth dilution. Neely (1977) estimates the rate constant for uptake of a chemical by a fish as a function of the volume of water flowing past the gills, the efficiency of pollutant transfer across the gills and the weight of the fish. Fulkerson et al. (1974) estimates the rate of solute uptake by a plant from the soil as a function of root biomass.

SUMMARY

The available models for predicting fluxes at the interfaces are summarized in Table III according to the criteria presented in the Introduction. The models have potential applicability for a wide variety of soils, vegetation, aquatic animals and pollutants. Input data are most readily available for modeling the interface with air, and only for this interface has some validation and sensitivity analysis been done to assess the models' actual applicability.

TABLE III

EVALUATION OF INTERFACE MODELS

Type of Model	Applicability	Accuracy, Validation	Input Data Available	Assumptions	Sensitivity Analysis	Cost
Air to Water/ Soil Interface	Covers many types of soil, pollutants.	Some com- parisons with field data.	Meteorolo- gical data available. Other fac- tors usually must be measured.	Explained.	Done for key factors.	Un- known.
Soil to Water Interface	Organic compounds, some models for heavy metals	Field data used for calibration, not yet enough for validation.	Available for simplest models only.	Explained.	Not extensive.	Un- known.
Uptake by Biological Systems	Wide appli- cability possible.	Some com- parisons with field data.	Not readily available.	Explained.	Not done.	Un- known.

SECTION VI

EXAMPLES OF FATE MODELS

An overall model of the environmental fate of a substance could be constructed by sequentially linking single-medium models using the equations describing the processes at the interfaces that have been presented in the preceding sections. An example of such a model is the Unified Transport Model developed at the Oak Ridge National Laboratory. Several other theoretical models of environmental fate have also been described, although their applications have been limited to a single medium.

UNIFIED TRANSPORT MODEL

A team of researchers at the Oak Ridge National Laboratory has developed a system of models whose purpose is to simulate the movement of a trace contaminant in and through a watershed. In concept, submodels that simulate the transport and fate of the substance in a single medium can be linked together using other submodels which simulate activity at the interfaces. The coupled submodels are called the Unified Transport Model. Several examples of the models describing the interfaces have been referred to previously in this report. The following sections describe the overall model, its development and applications.

Theory

The Unified Transport Model (UTM) is a physically based model designed to simulate the transport, accumulation and redistribution of trace contaminants in the environment. The air, land, and aquatic systems are represented by three major model components, designed to be run in sequence. The focus of the UTM has been on watershed phenomena that are important in trace contaminant mobility and pathways including atmospheric dispersion, deposition on land, entrainment and erosion in over-land flow, movement and exchange of soluble chemical species with the moisture flux through the soil matrix, transport in the stream channel and exchange with the stream sediment. Recent refinements of the model have included chemistry of sulfur in the atmosphere, sediment transport and soil chemistry along with

plant uptake and vegetative growth. These additions extend the purely physical framework to include some ecological processes.

The development of the UTM began with a search for existing models that could be modified to provide appropriate data to be run sequentially. The process of linking is complicated by differences in scale and accuracy between the various media models. Differences in scale reflect not only the state-of-the-art of modeling but also the inherent differences in processes which are important in the various media. Considerable time was spent making the necessary compromises.

Fulkerson et al. (1974) describes the sources of the models and the modifications. No comprehensive models were available for sediment transport, plant uptake and atmospheric chemistry; the new models developed for these phenomena at Oak Ridge are described by Van Hook and Shults (1976).

Designed for flexibility in a wide variety of applications, the UTM is actually a collection of compatible but distinct, stand-alone submodels. Figure 1 illustrates the suite of submodels that may be used in assembling a model to address a specific problem. The aim has been to reduce the complexity of the modeling system required for a particular problem, thereby reducing resource costs and increasing user understanding of the results.

As the UTM has become more detailed, individual submodels have been divided into subroutines representing specific physical processes; users should thus be better able to understand the functioning of the model and to make substitutions for particular algorithms. In addition, this type of structure can be modified as the state-of-the-art advances or reassembled for special applications not necessarily foreseen in the original formulation.

Applications and Validation

Two watersheds, Walker Branch and Crooked Creek, have been the focus of applications of various versions of the UTM and its submodels. Data from these watersheds have been collected for the specific purpose of validating these models. The air transport submodel (ATM) has been used to estimate deposition and air concentration of some 19 trace metals present in the Walker Branch watershed near Oak Ridge, Tennessee. For 16 of the metals, the simulated results were within the measured concentration ranges. The hydrology transport model (WHTM) estimated stream flows for the summers fairly well in this area but underestimated the heavier winter and spring flows. The hydrology transport model was also applied using the optimization routine (OPTRM), which provided simulated results closer to the measured values.

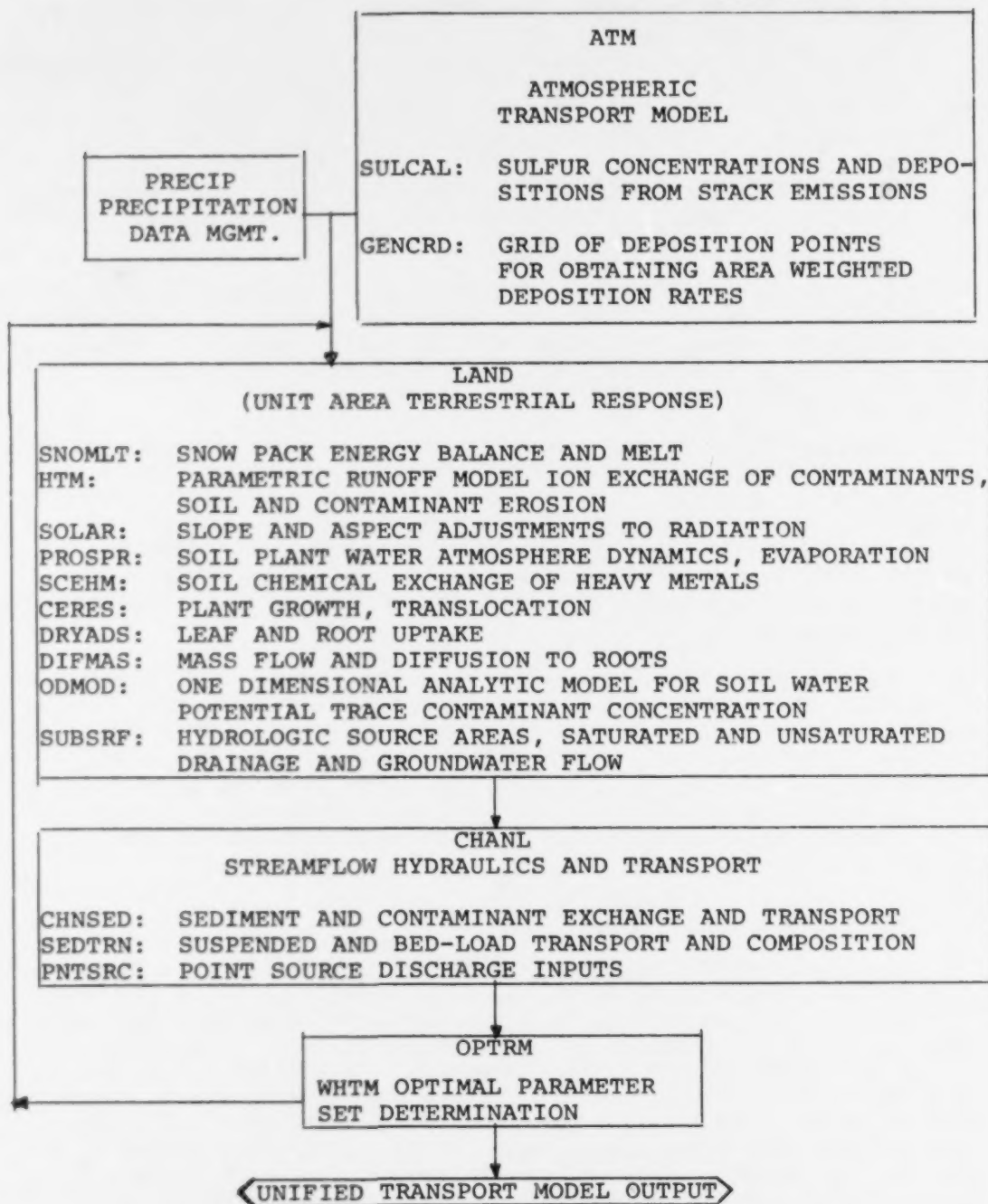


Figure 1. The submodels that may be linked to form a unified transport model.

Source: Van Hook and Shults (1976), p. 16.

In the Crooked Creek watershed in Missouri, the UTM has been used to model the fate of various metals. Two different versions of the model, both with the same air (ATM) and stream channel routing systems, but with different submodels (WHTM or TEHM) for the land portion of the system, have been developed. WHTM uses considerably less input data and simulates water quality of streams and buildup of toxic substances in the soil. TEHM provides additional information on the effects of toxic metals on plant growth and their accumulation in plant materials. Runs of these two versions of UTM are compared to each other as well as to measured data (Munro et al., 1976) in order to discover remaining problems in the formulation of the model.

These problems include the estimated rate of deposition (too low), the lack of differentiation between complexed and free heavy metals (the model predicts best those metals remaining as free cations in the soil solution), and the lack of sufficient input data to adequately characterize the system (sensitive parameters must be estimated).

Input

The input requirements will, of course, depend on the particular problem and set of models used. Table IV lists the input data required for the two major components of the UTM.

Sensitivity Analysis

Some submodels have been subjected to various sensitivity analyses. Usually a series of calculations is made to show how various output quantities change as input quantities are varied in ranges thought to be realistic. These sensitivity analyses serve several functions. First, many input items are hard to measure. One of the submodels (OPTRM) was developed to optimize or search for the best parameter values for the particular application. This calibrates the model to the specific watershed being studied. The sensitivity of the simulated variable to various parameters guides the choice of the set of parameters to be optimized. Second, researchers often use the model in developing and testing hypotheses. Changes in output values point to which pathways or processes may be dominant for any given situation. Third, when input data are unavailable for a particular application, they may be estimated from the results of the sensitivity studies.

Cost and Documentation

Each submodel has been well documented. The documentation generally includes a description of the input data required, where it was obtained by the researchers, the structural equations used, a flow diagram, the FORTRAN IV listing, an example of the output produced and a description of applications of the

TABLE IV
INPUT REQUIREMENTS AND OUTPUT DATA
FOR TWO COMPONENTS OF THE UNIFIED TRANSPORT MODEL

ATMOSPHERIC TRANSPORT MODEL

INPUT: type of material (particle or gas), density, size, wind speeds, wind directions, atmospheric stability, geographic location, type and strength of emission sources, height of stack, plume rise factor, hourly precipitation

OUTPUT: wet and dry deposition amounts, surface concentration

WISCONSIN HYDROLOGIC TRANSPORT MODEL

INPUT: hourly precipitation, daily maximum and minimum temperatures, daily pan evaporation rates, hourly temperature and humidity, daily precipitation, solar radiation; upper and lower zone soil storage, soil moisture evaporation index, time distribution parameter for interflow, average length of overland flow, average slope of overland flow plane, interflow recession constant, groundwater recession parameter, impervious area and other parameters describing land features; residual toxicant mass distributed on land surface, ion-exchange distribution coefficient, deposition amounts, toxicant content of ion exchange plates and other parameters describing toxicant properties.

OUTPUT: daily stream flow, total metal transported, daily average metal concentration

Abstracted from Munro (1976).

model. In addition, Van Hook and Shults (1976) briefly describe some of the steps in implementing the model that may prove costly and time-consuming.

CONCEPTUAL MODEL

Ecosystem modeling has been characterized by the collection of voluminous but not always relevant data. Although the environmental fate of some compounds (primarily pesticides, e.g. DDT) has been successfully modeled in this way, it is a highly inefficient hit-or-miss method. Thousands of chemicals are now manufactured, used and ultimately disposed of in the environment. Managing the dispersal of these chemicals would be easier if there were simpler, more reliable ways of evaluating their potential hazard. An explicit model derived from the principles of chemistry, physics and biology and valid for all chemicals and all environments is not possible given the bounds of current knowledge.

Instead a procedure for deriving a conceptual model for the movement of chemicals through the environment is proposed by Gillett et al. (1974). The purpose of this model is to force rigorous thinking about what processes and components of the environment are involved. The conceptual model starts with a diagrammatic representation of the processes and components and their possible interactions. For instance, if the flow of a pesticide through a terrestrial system is being investigated, the components would include biota and soil and the processes would include volatilization from soil, adsorption-desorption onto soil and loss to biota, among others.

The model is refined through an iterative process of reduction and expansion of components. In examining the effect of root growth on the physical structure of the soil, for instance, the biota component might be divided into root and stem systems or the soil into several layers. If it turned out that this expansion of the model did not alter the pattern of movement of the pesticide through the soil, then the model could be reduced. The root and stem components could be recombined into one biota component or the number of soil layers could be reduced without affecting the capacity of the model to predict pesticide transport.

Another example of the iterative process of reduction and expansion will be presented more fully below in the discussion of the environmental rates approach. Briefly, this procedure evaluates process-system interactions, providing criteria for the elimination of components that have the least effect on system behavior. The operation of the thus simplified model may in turn point out other components that should be expanded to model the particular problem more adequately.

The aim is to put bounds on the types of measurements needed, the accuracy required of the measurements and the frequency of sampling. An example of this procedure is given by Haefner and Gillett (1976). This approach is still in the conceptual stage, with current efforts focused on deriving a functional mathematical statement for simulation experiments and better defining measurement needs.

MASS BALANCE APPROACH

A mass balance study essentially accounts for all sources, pathways, transformations and sinks for a particular pollutant in a given area. The mass balance approach traces the flow of a pollutant through an area. Each environmental pathway is characterized as a chemical, physical or ecological interaction and by a mass flow rate. The assumption is that the flow rates can be estimated separately. Then the analysis requires a satisfactory mass balance; that is, the sum of input flows should equal the sum of output flows and stored quantities. This approach can be applied to all substances and media as long as the important environmental processes and input and output characteristics are known.

Huntzicker et al. (1975) reports on applications of this methodology in the Los Angeles area. Applications have been primarily limited to determining fate of airborne trace metal pollutants. The input, flow rate and output data required for this type of analysis are shown in Table V. Problems encountered in these examples include an inaccurate emissions inventory resulting in uncertain input flows as well as a lack of theoretical or experimental understanding of particular removal processes in the environment. Given these uncertainties and the large geographical expanse of the study areas, the method does not provide detailed predictions of pollutant dispersion. It does provide estimates of the relative flow of mass for each source and sink identified.

Most of the studies are site-specific (e.g., Los Angeles air basin); most model substances currently being emitted into the atmosphere and use data collected in the field. However, one study forecasts the flow of manganese as a substitute for lead in gasoline. Because field data for this new substance were not available, input data were estimated from lead flows, because the two substances have similar particle size distributions in automobile exhaust.

A similar approach to forecasting the fate of substances not widely dispersed in the environment is described in the next section. The materials balance equations are still used but the source of flow rates differ. Also, the primary emphasis

TABLE V
MASS BALANCE APPROACH
EXAMPLE OF INPUT AND OUTPUT DATA
FOR AIRBORNE TRACE METAL POLLUTANTS

Source or Input Data

1. Identity of sources
2. Mass emission rates for each source
3. Aerosol size distribution for each source
4. Deposition rate (dry)
5. Rainout-washout rate (wet)

Output Data

1. Atmospheric flushing (ventilation) rates
 - a. Receptor site atmospheric concentration
 - b. Volumetric flow through air basin
2. Inputs to coastal waters, lakes, rivers, etc.
 - a. Deposition (dry)
 - b. Rainout-washout
 - c. Runoff
 - d. Sewage

Source: J. Huntzicker, S. Friedlander and C. Davidson (1975), p. 5.

has been on applications in aquatic environments rather than in the atmosphere.

ENVIRONMENTAL RATES APPROACH

This approach to predicting the fate of a substance in the environment uses the results of laboratory measurements of specific physical, chemical and biological processes in a computer model that integrates the data with transport parameters. The laboratory data are collected in the form of rate constants. These rate constants are then used in the material balance models to produce time-varying concentrations. All of the rate processes are described by expressions involving a term for concentration, and each rate is a function of some property of the environment such as pH, turbulence, and light intensity. This approach essentially considers what the environment does to the substance rather than the reverse. Thus, the importance of environmental pathways corresponding to a particular process is determined by its effect on the net rate of loss or accumulation of the substance.

The temptation in seeking to eliminate the least important variables is to focus on very rapid processes (which cannot be rate limiting) and on very slow processes (which cannot transport must matter). However, the environmental rates approach shows that the effect of a process is dependent on other factors as well as the rate coefficient and provides a technique for estimating this effect.

The fundamental assumptions on which this approach is based are that

- (1) the overall rate of disappearance of a substance is controlled by the dominant transformation and transport processes,
- (2) these processes can be studied separately in the laboratory, and
- (3) the laboratory data can be extrapolated to environmental conditions.

Unlike the site-specific transport models we have discussed earlier, this approach hypothesizes an idealized environment. It can evaluate the influence of properties of the environment by varying these properties and recording the resulting variation in the fate of the substance. Thus, the input data are usually specified rather than measured. This approach permits generalizations based on both chemical and environmental properties. It is not intended to predict detailed fate in specific environments, but the results can be used to

assess the need for more detailed studies. This lack of specificity is not necessarily a disadvantage. Where new substances have not yet been introduced into the environment, it is still possible to study their probable fate or at least to determine what further tests are needed. Also, for substances that are not widely dispersed and for which the collection or monitoring or field data may not be practical, this approach could be used to allocate monitoring resources more efficiently.

The environmental rates approach predicts concentrations as a function of time. The usual model ecosystem studies, in contrast, report equilibrium or single time values. Although microcosm studies yield an overall assessment of complex interactions in an environment, they do not provide a basis for extrapolation. The environmental rates method, by providing relative rates of many processes, provides a basis for extrapolation and a fundamental understanding of what happened to the substance.

Output

Several kinds of results can be obtained from this type of model. First, the distribution within the environment for given source characteristics is given in the form of concentration or mass of the pollutant. Steady-state concentrations are measures of exposure for organisms living in the aquatic environment. Second, dominant pathways are found as a function of the environment's properties. If the products that result from a particular transformation are known, then examination of the dominant pathways will identify what products should be present. Third, the model can be used for ranking chemicals from the point of view of chronic exposure. Together with toxicity data the predicted concentrations could be used to produce relative hazard rankings. Fourth, the relative patterns of concentration in different parts of the environment may suggest areas that need further study. If a chemical largely dissipates into the atmosphere, then photo-degradation studies are indicated. On the other hand, if there seems to be an accumulation in fish, fish metabolism might be studied.

Validation

Knowledge of environmental processes and methods for predicting their rates is not extensive. Research by Smith et al. (1977) has focused on this problem for the aquatic environment. The principles, however, are applicable for any compound or medium. A potential weakness of this approach is that it may not incorporate all important transport or transformation processes that occur in a natural system. Thus, validation of this model should be done by comparing concentrations in laboratory microcosms or, if possible, natural systems. This sort of validation cannot prove that the model includes all

important processes. There is no way to test this mechanically. However, it can show the model to be inadequate in comparison with the experimental or field data and that further model development is needed.

Operational models incorporating this approach are few. One of the earliest was an application to air pollution (Friedlander and Seinfeld, 1969). More recently, they have been applied to transport and transformation of substances in water. Hill et al. (1976) examines the behavior of vinyl chloride and Lassiter et al. (1976) describes the fate of mercury. Neely (1977) presents a computer program for predicting environmental exposure concentrations of a neutral organic chemical. This model has been constructed so as to require as a minimum data base, the aqueous solubility, the vapor pressure and molecular weight of the chemical. It will then generate rate constants for characterizing the various movements of the chemical from water to soil, to air and to fish. Smith et al. (1977) describes a compartmental model of a freshwater environment incorporating the transport and transformation processes studied in the laboratory, the laboratory procedures they have developed for measuring the rate constants and the results of using this model to study eleven chemicals.

Applications of this method has not been extensive, and there are few material balance studies in the field to be used in verification of this approach. Also, some of the assumptions explicit in the models are poorly substantiated or understood at this time; further applications might provide insights into their consequences or limitations.

Input

Rate constants for the processes included in any particular application are estimated in the laboratory. Smith et al. (1977) describes how this is done for physical (solubility in water, absorption spectra, volatilization, sorption partition coefficients), chemical (photolysis, free radical oxidation, hydrolysis) and biological (biodegradability) properties of an aquatic environment. Neely (1977) describes how to estimate the evaporation rate constant, soil uptake, soil release, fish uptake and fish excretion from basic properties of the system if experimental data are not available.

Sensitivity Analysis

Branson (1977) presents results obtained by varying some of the rate constants. The hydrolysis rate, bioconcentration uptake rate and water solubility are varied by approximately $\pm 10\%$ and compared to the resulting variation in concentration of the substance in fish and in water.

SUMMARY OF FATE MODEL FINDINGS

The environmental fate models described in this report could theoretically be applied to a variety of environmental conditions and types of pollutants. However, in practice their applications are limited. Sensitivity analyses have been performed for several models, prompted primarily by the lack of available input data. Through sensitivity analysis it is possible to determine which kinds of inaccuracy in the input data significantly influence the output results and which are less important. Table VI presents a summary description of these fate models according to the criteria listed in the introduction to this report.

No matter how sophisticated modeling becomes, an understanding of environmental fate and predominant pathways alone cannot be a sufficient guide to potential risk. For instance, it might be established that a substance volatilizes rapidly, implying that the largest concentrations will be found in the air medium. However, if investigation were limited to its chemical transformations and transport in air, its highly toxic properties at very low concentrations in water might be overlooked.

TABLE VI

EVALUATION OF FATE MODELS

Type of Model	Applicability	Accuracy, Validation	Input Data Available	Assumptions	Sensitivity Analysis	Cost
Unified Transport Model	Transport of heavy metals in all media.	Two applications and comparisons with field data.	Large amount of data required, some not readily available.	Well documented.	Done for key factors, has optimization routine.	Described.
Conceptual Model	Wide applicability possible.	No applications.	Unknown.	Would be described for each application.	None.	Unknown.
Mass Balance Approach	Wide applicability possible.	Applications for trace metals in air; comparisons with field data.	Available but emission rates not very accurate.	Explained.	Done for input emission rates.	Unknown.
Environmental Rates Approach	Wide applicability possible.	Applications for organic compounds in aquatic systems.	Available from laboratory measurements.	Well documented.	Not extensive.	Unknown.

SECTION VII

EXAMPLES OF EXPOSURE ASSESSMENTS

The previous sections have described the development of models to estimate pollutant concentrations, exposure and effects relationships and size of exposed population. However, few quantitative exposure assessments have actually been made.

An ideal model applicable to most substances would include:

- provision for multiple emission sources
- conversion of emission rates to contaminant concentrations in all media (air, water, soil, food)
- provision for exposure to humans, plants and animals
- provision for multiple routes of exposure to humans (inhalation, ingestion, transpiration)
- allowance for interactive effects (synergistic or antagonistic) of multiple pollutants.

Our review of the models developed so far suggests that we cannot expect to discover a well-developed, operational exposure assessment model meeting all these conditions. Nevertheless, regulatory decisions must be made and exposure or risk assessments have been done. Table VII summarizes several such risk assessment studies.

These studies have concentrated on human health effects, air pollutants, exposure through inhalation only, and one pollutant without accounting for synergistic effects. Although some do propose methodologies to cover multiple exposure routes and media, their applications revert to single exposure routes and media because the data necessary to extend the analysis are not available. In addition, only a few of the studies address the problems of accuracy, validation and sensitivity analysis. No study states its cost.

However, each study does provide at a minimum estimates for size of exposed population, exposure level and resultant risk. Differences in the available input data and the purpose of the analysis have led to different methods of calculating risk. It appears possible that estimates of accuracy, even if only as orders of magnitude, and sensitivity analyses of dose-response assumptions could have been made in most instances.

TABLE VII

RISK ASSESSMENT STUDIES

Reference	Model Type Assumptions	Input Data	Output Data	Accuracy	Validation	Sensitivity Analysis
Kuzmack and McGaughy (1976)	Links exposure, concentrations and effects. Vinyl chloride. Inhalation route only.	Size of population. Air diffusion model. No. and location of emission sources.	Cases of illness per year of exposure	-10% to +55%	Compares animal study results to human data	Different dose-response curves used.
Albert (in draft)	Links studies of exposure and effects. Benzene. Inhalation route only.	Linear, non-threshold dose-response model. Production data. Dispersion model. Population density. Epidemiological studies.	For various sources of benzene: lifetime risk, expected no. of cases per year	Several orders of magnitude	Compares to results to occupational study.	None
Albert (1977)	Census study of farm workers exposed to herbicides. Assumes all inhaled is absorbed. Inhalation route only.	Monitoring data on concentration levels. Survey estimates of exposure. Animal studies for dose-response.	No. of cases of cancer from lifetime exposure for various types of control programs.	Considerable uncertainty.	None	None

TABLE VII - continued

Reference	Model Type Assumptions	Input Data	Output Data	Accuracy	Validation	Sensitivity Analysis
EPA (1977)	Link emissions to concentration to exposure to effects. For cadmium and asbestos. Includes sources from air, water, food & tobacco.	Emission rate, background concentration in food, body burden model, dose response curves, population density and mobility.	Decrease in life expectancy. Rate of illness.	Confidence limits for input data & dose-response curves.	None	None
Finklea et al. (1977)	Links census data to air monitoring data for air pollutants. Assumes best judgment threshold for dose-response curves.	Census population data. Air monitoring data. Dose response curves.	Excess deaths. Excess days of illness per susceptible population groups due to not meeting standards.	Qualitative statements of uncertainty.	Compares best judgment thresholds to least squares fit.	None
Walsh et al. (1977)	Sums over exposure routes (air, water, food) for total body dose. Theory covers multiple pollutants but data does not.	Transport models. Physiologic models of uptake.	Index of dose divided by safe limit. Effluent limit so as not to exceed safe limit.	Depends on input models.	Depends on input models.	None

SECTION VIII

OTHER USES FOR THE MODELS

The risk assessments discussed above concern pollutants that are present in the environment and many of the environmental fate models depend on measurements done in the field. A major source of uncertainty in the applications of these models is the lack of measurements for input data. These models can be used, then, to indicate what input data are needed but not now routinely collected. A conceptual framework, called Integrated Exposure Assessment Monitoring, has been proposed which in conjunction with these models would optimize collection of these data.

Resources for monitoring and modeling, however, are not unlimited. Ranking (screening, indexing) schemes have been proposed to set priorities among substances needing EPA regulatory attention. Modeling can be useful in evaluating the hazards posed by substances already dispersed in the environment or the potential risks in new substances being proposed for use.

These two uses of exposure assessment data are discussed briefly below.

INTEGRATED EXPOSURE ASSESSMENT MONITORING

Integrated Exposure Assessment Monitoring is a concept being developed by EPA's Environmental Monitoring and Support Laboratory in Las Vegas. It provides a framework for the systematic collection and coordination of pollution data in air, water, land and food. The idea is to optimize the use of monitoring resources by focusing on measurements that are directly related to critical receptors (the sub-group of humans, animals or plants showing effects at a dose lower than any other group) and critical sources (major contributors to exposure of the critical receptors). This approach differs from past EPA monitoring efforts by focusing on total exposure to a pollutant rather than on exposure from a single medium. Current EPA monitoring systems involve single-medium trend monitoring or source monitoring. This type of data is not adequate to address the problems of acute or chronic health effects that may result from short-term peak exposure, repeated short-term high exposures or low-level,

long-term exposures, or the problem of synergism or the latency period between exposure and illness. Current monitoring systems measure intensity in one medium only and thus cannot generally be related to other media. Data identifying environmental characteristics, pathways, chemical and physical form, frequency, duration and intensity are needed for an exposure assessment.

The exposure assessment monitoring concept has been applied to lead. Jenkins (1976) finds that in spite of the voluminous data available on the distribution and effects of lead, the information is generally not in a form that can be used to quantify the contribution of sources and pathways. He then investigates what mathematical models might be available to translate measurable data into information appropriate for a total exposure assessment. Such models can be of value in helping identify the relative importance of various sources, pathways and exposure routes. Pollutant transport and transformation models as well as models for distribution of lead in the body were investigated. The result of this analysis was to show the use and limitations of currently available data and the relative importance of obtaining various kinds of required missing data.

This approach, then, provides a framework for logically organizing existing information and determining what kinds of missing information are needed. However, the lack of appropriate data and models hinders the actual operation of such a system. The approach has several other pertinent limitations. Each pollutant would potentially require a different monitoring system. Control of the critical source, as here defined, may not necessarily eliminate the effect in question. Finally, the focus on critical receptors does not define an overall population exposure or risk.

RANKING SCHEMES

Ranking schemes are used for priority ranking of environmental pollutants needing EPA regulatory attention. The same methodology used to rank suspected pollutants can also be used to evaluate the potential hazard of a substance not yet introduced into the environment, though in this case little information may be available. Because the decision-maker must initially decide just what types of information are important to him, every ranking scheme should explicitly list the information required.

Methods of organizing this information for use by the decision-maker range from a list subject to expert judgment through information screening and ordering to a formal model defining hazard.

A model-based system described by Brown and Holt (1976) would consist of six compartments to be modeled:

- 1) source: human and natural production
- 2) distribution: uses, disposal, releases to air, water, land
- 3) fate: transport, transformation, exposure
- 4) effects: dose-response relationships to estimate risk
- 5) valuation: assign value weights to effects
- 6) ranking: derive aggregate environmental hazard index and rank substances with respect to other substances.

The models discussed in this report would provide information for the fate and effects compartments.

SECTION IX

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